EXPECTATION VALUES IN RELATIVISTIC COULOMB PROBLEMS

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Abstract. We evaluate the matrix elements $\langle Or^p \rangle$, where $O = \{1, \beta, i\boldsymbol{\alpha}\mathbf{n}\beta\}$ are the standard Dirac matrix operators and the angular brackets denote the quantum-mechanical average for the relativistic Coulomb problem, in terms of generalized hypergeometric functions ${}_3F_2(1)$ for all suitable powers. Their connections with the Chebyshev and Hahn polynomials of a discrete variable are emphasized. As a result, we derive two sets of Pasternack-type matrix identities for these integrals, when $p \to -p-1$ and $p \to -p-3$, respectively. Some applications to the theory of hydrogenlike relativistic systems are reviewed.

1. Introduction

Recent experimental progress has renewed interest in quantum electrodynamics of atomic hydrogenlike systems. Experimentalists and theorists in atomic and particle physics are discovering problems of common interest with new ideas and methods. A current account of the status of this fundamental area of quantum physics, which is more than a century old, is given in Refs. [29], [30], [38], and [58]. Exciting research topics vary from experimental testing of Quantum Electrodynamics (QED) to fruitful training models for the bound-state Quantum Chromodynamics and Bose–Einstein Condensation [14], [29], [30], [31], [38], [58], and [63].

The highly charged ions are an ideal testing ground for the strong-field bound-state QED. They posses a strong static Coulomb field of the nucleus and a simple electronic structure which can be accurately computed from first principles. It is possible nowadays to make massive highly charged ions with a strong nuclear charge and only one electron through the periodic table up to uranium, the most highly charged ion [26], [27]. These systems are truly relativistic and require the Dirac wave equation as a starting point in a detailed investigation of their spectra [38], [55]. The binding energy of a single K-shell electron in the electric field of a uranium nucleus corresponds to roughly one third of the electron rest mass. For the simple hydrogen atom the nonrelativistic Schrödinger approximation can be used [8].

For the last decade, the two-time Green's function method of deriving formal expressions for the energy shift of a bound-state level of high-Z few-electron systems was developed [55] and numerical calculations of QED effects in heavy ions were performed with excellent agreement to current experimental data [26], [27] (see [52], [53], [54], [57], [58], and [63] and references therein for more details). These advances motivate, among other technical things, evaluation of the expectation values $\langle Or^p \rangle$ for the standard Dirac matrix operators $O = \{1, \beta, i\boldsymbol{\alpha}\mathbf{n}\beta\}$ between the bound-state relativistic Coulomb wave functions. Special cases appear in calculations of the magnetic dipole

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hyperfine splitting, the electric quadrupole hyperfine splitting, the anomalous Zeeman effect, and the relativistic recoil corrections in hydrogenlike ions (see, for example, [1], [56], and [54] and references therein). We discuss convenient closed forms of these integrals in general and derive matrix symmetry relations among them which can be useful in the theory of relativistic Coulomb systems.

The paper is organized as follows. In the next section we review the relativistic Coulomb wave functions and set up the notations. The expectation values $\langle Or^p\rangle$ are evaluated in section 3 in terms of the generalized hypergeometric functions ${}_3F_2\left(1\right)$ for all admissible powers of r. Their Pasternack-type matrix symmetry relations are established in section 4 and recurrence relations are given in section 5. We discuss special matrix elements and review some of their applications in the last section. An attempt to collect the available literature is made. The appendix A contains definition of the generalized hypergeometric series and proof of a required transformation identity. The appendix B deals with the Dirac matrices and inner product.

2. Wave Functions for the Relativistic Coulomb Problem

The exact solutions of the stationary Dirac equation

$$H\psi = \left(c\boldsymbol{\alpha}\mathbf{p} + mc^2\beta - Ze^2/r\right)\psi = E\psi \tag{2.1}$$

for the Coulomb potential can be obtained in the spherical coordinates. The energy levels were discovered in 1916 by Sommerfeld [59] from the "old" quantum theory and the corresponding (bispinor) Dirac wave functions were found later by Darwin [16] and Gordon [25] at the early age of discovery of the "new" wave mechanics (see also [9] for a modern discussion of "Sommerfeld's puzzle"). These classical results are nowadays included in all textbooks on relativistic quantum mechanics, quantum field theory and advanced texts on mathematical physics (see, for example, [2], [7], [8], [28], [37], and [40]). The end result is

$$\psi = \begin{pmatrix} \boldsymbol{\varphi} \\ \boldsymbol{\chi} \end{pmatrix} = \begin{pmatrix} \mathcal{Y}_{jm}^{\pm}\left(\mathbf{n}\right)\ F\left(r\right) \\ i\mathcal{Y}_{jm}^{\mp}\left(\mathbf{n}\right)\ G\left(r\right) \end{pmatrix}, \tag{2.2}$$

where the spinor spherical harmonics $\mathcal{Y}_{jm}^{\pm}\left(\mathbf{n}\right) = \mathcal{Y}_{jm}^{(j\pm1/2)}\left(\mathbf{n}\right)$ are given explicitly in terms of the ordinary spherical functions $Y_{lm}\left(\mathbf{n}\right)$, $\mathbf{n} = \mathbf{n}\left(\theta,\varphi\right) = \mathbf{r}/r$ and the special Clebsch–Gordan coefficients with the spin 1/2 as follows [2], [7], [46], [61]:

$$\mathcal{Y}_{jm}^{\pm}\left(\mathbf{n}\right) = \begin{pmatrix} \mp\sqrt{\dfrac{\left(j+1/2\right)\mp\left(m-1/2\right)}{2j+\left(1\pm1\right)}}\ Y_{j\pm1/2,\ m-1/2}\left(\mathbf{n}\right) \\ \sqrt{\dfrac{\left(j+1/2\right)\pm\left(m+1/2\right)}{2j+\left(1\pm1\right)}}\ Y_{j\pm1/2,\ m+1/2}\left(\mathbf{n}\right) \end{pmatrix} \tag{2.3}$$

with the total angular momentum $j = 1/2, 3/2, 5/2,\ ...$ and its projection $m = -j, -j+1,\ ..., j-1, j$ (see also Section VI A of Ref. [60] for the properties of the spinor spherical harmonics).

The radial functions $F\left(r\right)$ and $G\left(r\right)$ can be presented as [40]

$$\begin{pmatrix} F\left(r\right) \\ G\left(r\right) \end{pmatrix} = \frac{a^2\beta^{3/2}}{\nu}\sqrt{\frac{\left(\varepsilon\kappa-\nu\right)n!}{\mu\left(\kappa-\nu\right)\Gamma\left(n+2\nu\right)}}\ \xi^{\nu-1}e^{-\xi/2}$$

$$\times \begin{pmatrix} f_1 & f_2 \\ g_1 & g_2 \end{pmatrix} \begin{pmatrix} \xi L_{n-1}^{2\nu+1}(\xi) \\ L_n^{2\nu-1}(\xi) \end{pmatrix}. \tag{2.4}$$

Here, $L_k^\alpha(\xi)$ are the Laguerre polynomials given by (A.2) and we use the following notations:

$$\kappa = \pm (j+1/2), \qquad \nu = \sqrt{\kappa^2-\mu^2}, \qquad \mu = \alpha Z = Ze^2/\hbar c, \tag{2.5}$$
$$a = \sqrt{1-\varepsilon^2}, \qquad \varepsilon = E/mc^2, \qquad \beta = mc/\hbar = 1/\lambda,$$

and

$$\xi = 2a\beta r = 2\sqrt{1-\varepsilon^2}\,\frac{mc}{\hbar}\,r. \tag{2.6}$$

The elements of 2×2–transition matrix in (2.4) are given by

$$f_1 = \frac{a\mu}{\varepsilon\kappa-\nu}, \quad f_2 = \kappa-\nu, \quad g_1 = \frac{a(\kappa-\nu)}{\varepsilon\kappa-\nu}, \quad g_2 = \mu. \tag{2.7}$$

This particular form of the relativistic radial functions is due to Nikiforov and Uvarov [40]; it is very convenient for taking the nonrelativistic limit $c\to\infty$ (see also [60]).

The relativistic discrete energy levels $\varepsilon = \varepsilon_n = E_n/E_0$ with the rest mass energy $E_0 = mc^2$ are given by the Sommerfeld–Dirac fine structure formula

$$E_n = \frac{mc^2}{\sqrt{1+\mu^2/(n+\nu)^2}}. \tag{2.8}$$

Here, $n = n_r = 0, 1, 2, \ ...$ is the radial quantum number and $\kappa = \pm(j+1/2) = \pm 1, \pm 2, \pm 3, \ ...$. The following identities

$$\varepsilon\mu = a(\nu+n), \quad \varepsilon\mu + a\nu = a(n+2\nu), \quad \varepsilon\mu - a\nu = an, \tag{2.9}$$
$$\varepsilon^2\kappa^2-\nu^2 = a^2 n(n+2\nu) = \mu^2 - a^2\kappa^2$$

are useful in calculation of the matrix elements below.

The familiar recurrence relations for the Laguerre polynomials allow to present the radial functions (2.4) in a traditional form [2], [7], [15], [34], [60] as follows

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = a^2\beta^{3/2}\sqrt{\frac{n!}{\mu(\kappa-\nu)(\varepsilon\kappa-\nu)\Gamma(n+2\nu)}}\,\xi^{\nu-1}e^{-\xi/2} \tag{2.10}$$
$$\times \begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix} \begin{pmatrix} L_{n-1}^{2\nu}(\xi) \\ L_n^{2\nu}(\xi) \end{pmatrix},$$

where

$$\alpha_1 = \sqrt{1+\varepsilon}\left((\kappa-\nu)\sqrt{1+\varepsilon}+\mu\sqrt{1-\varepsilon}\right), \quad \alpha_2 = -\sqrt{1+\varepsilon}\left((\kappa-\nu)\sqrt{1+\varepsilon}-\mu\sqrt{1-\varepsilon}\right), \tag{2.11}$$

$$\beta_1 = \sqrt{1-\varepsilon}\left((\kappa-\nu)\sqrt{1+\varepsilon}+\mu\sqrt{1-\varepsilon}\right), \quad \beta_2 = \sqrt{1-\varepsilon}\left((\kappa-\nu)\sqrt{1+\varepsilon}-\mu\sqrt{1-\varepsilon}\right) \tag{2.12}$$

and a convenient identity holds

$$\left((\kappa-\nu)\sqrt{1+\varepsilon}\pm\mu\sqrt{1-\varepsilon}\right)^2 = 2(\kappa-\nu)(\kappa-\nu\varepsilon\pm a\mu). \tag{2.13}$$

We give the explicit form of the radial wave functions (2.4) for the $1s_{1/2}$ state, when $n = n_r = 0$, $l = 0$, $j = 1/2$, and $\kappa = -1$:

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = \left(\frac{2Z}{a_0}\right)^{3/2} \sqrt{\frac{\nu_1 + 1}{2\Gamma(2\nu_1 + 1)}} \begin{pmatrix} -1 \\ \sqrt{\dfrac{1-\nu_1}{1+\nu_1}} \end{pmatrix} \xi_1^{\nu_1 - 1} e^{-\xi_1/2}. \tag{2.14}$$

Here, $\nu_1 = \sqrt{1-\mu^2} = \varepsilon_1$, $\xi_1 = 2\sqrt{1-\varepsilon_1^2}\beta r = 2Z(r/a_0)$, and $a_0 = \hbar^2/me^2$ is the Bohr radius. One can see also [2], [7], [8], [16], [19], [25], [28], [34], [37], and [50] and references therein for more information on the relativistic Coulomb problem.

3. Evaluation of the Matrix Elements

We evaluate the following integrals of the radial functions:

$$A_p = \int_0^\infty r^{p+2} \left(F^2(r) + G^2(r)\right) \, dr, \tag{3.1}$$

$$B_p = \int_0^\infty r^{p+2} \left(F^2(r) - G^2(r)\right) \, dr, \tag{3.2}$$

$$C_p = \int_0^\infty r^{p+2} F(r) G(r) \, dr \tag{3.3}$$

in terms of generalized hypergeometric series. (Their relations with the expectation values of the operators $\langle O r^p \rangle$, where $O = \{1, \beta, i\boldsymbol{\alpha}\mathbf{n}\beta\}$, are discussed in the appendix B.) The final results with the notations from the previous section can be presented in two different closed forms. Use of the traditional radial functions (2.10) results in:

$$\begin{aligned} 2\mu (2a\beta)^p \, \frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)} \, A_p &= 2p\varepsilon a n \; {}_3F_2\left(\begin{matrix} 1-n, \; -p, \; p+1 \\ 2\nu+1, \quad 2 \end{matrix}\right) \\ &+ (\mu + a\kappa) \; {}_3F_2\left(\begin{matrix} 1-n, \; -p, \; p+1 \\ 2\nu+1, \quad 1 \end{matrix}\right) + (\mu - a\kappa) \; {}_3F_2\left(\begin{matrix} -n, \; -p, \; p+1 \\ 2\nu+1, \quad 1 \end{matrix}\right), \end{aligned} \tag{3.4}$$

$$\begin{aligned} 2\mu (2a\beta)^p \, \frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)} \, B_p &= 2pan \; {}_3F_2\left(\begin{matrix} 1-n, \; -p, \; p+1 \\ 2\nu+1, \quad 2 \end{matrix}\right) \\ &+ \varepsilon (\mu + a\kappa) \; {}_3F_2\left(\begin{matrix} 1-n, \; -p, \; p+1 \\ 2\nu+1, \quad 1 \end{matrix}\right) + \varepsilon (\mu - a\kappa) \; {}_3F_2\left(\begin{matrix} -n, \; -p, \; p+1 \\ 2\nu+1, \quad 1 \end{matrix}\right), \end{aligned} \tag{3.5}$$

$$\begin{aligned} &4\mu (2a\beta)^p \, \frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)} \, C_p \\ &= a(\mu + a\kappa) \; {}_3F_2\left(\begin{matrix} 1-n, \; -p, \; p+1 \\ 2\nu+1, \quad 1 \end{matrix}\right) - a(\mu - a\kappa) \; {}_3F_2\left(\begin{matrix} -n, \; -p, \; p+1 \\ 2\nu+1, \quad 1 \end{matrix}\right). \end{aligned} \tag{3.6}$$

Nikiforov and Uvarov's form (2.4) gives the following result:

$$4\mu\nu^2 (2a\beta)^p \; A_p \tag{3.7}$$

$$
\begin{aligned}
&= a\kappa\left(\varepsilon\kappa+\nu\right)\frac{\Gamma\left(2\nu+p+3\right)}{\Gamma\left(2\nu+2\right)}\ {}_3F_2\left(\begin{array}{c} 1-n,\ p+2,\ -p-1 \\ 2\nu+2,\quad 1 \end{array}\right) \\
&-2\left(p+2\right)a^2\mu n\frac{\Gamma\left(2\nu+p+2\right)}{\Gamma\left(2\nu+1\right)}\ {}_3F_2\left(\begin{array}{c} 1-n,\ p+2,\ -p-1 \\ 2\nu+1,\quad 2 \end{array}\right) \\
&+a\kappa\left(\varepsilon\kappa-\nu\right)\frac{\Gamma\left(2\nu+p+1\right)}{\Gamma\left(2\nu\right)}\ {}_3F_2\left(\begin{array}{c} -n,\ p+2,\ -p-1 \\ 2\nu,\quad 1 \end{array}\right),
\end{aligned}
$$

$$
\begin{aligned}
&4\mu\nu\left(2a\beta\right)^p\ B_p \qquad (3.8)\\
&\quad = a\left(\varepsilon\kappa+\nu\right)\frac{\Gamma\left(2\nu+p+3\right)}{\Gamma\left(2\nu+2\right)}\ {}_3F_2\left(\begin{array}{c} 1-n,\ p+2,\ -p-1 \\ 2\nu+2,\quad 1 \end{array}\right) \\
&\quad -a\left(\varepsilon\kappa-\nu\right)\frac{\Gamma\left(2\nu+p+1\right)}{\Gamma\left(2\nu\right)}\ {}_3F_2\left(\begin{array}{c} -n,\ p+2,\ -p-1 \\ 2\nu,\quad 1 \end{array}\right),
\end{aligned}
$$

$$
\begin{aligned}
&8\mu\nu^2\left(2a\beta\right)^p\ C_p \qquad (3.9)\\
&\quad = a\mu\left(\varepsilon\kappa+\nu\right)\frac{\Gamma\left(2\nu+p+3\right)}{\Gamma\left(2\nu+2\right)}\ {}_3F_2\left(\begin{array}{c} 1-n,\ p+2,\ -p-1 \\ 2\nu+2,\quad 1 \end{array}\right) \\
&\quad -2\left(p+2\right)a^2\kappa n\frac{\Gamma\left(2\nu+p+2\right)}{\Gamma\left(2\nu+1\right)}\ {}_3F_2\left(\begin{array}{c} 1-n,\ p+2,\ -p-1 \\ 2\nu+1,\quad 2 \end{array}\right) \\
&\quad +a\mu\left(\varepsilon\kappa-\nu\right)\frac{\Gamma\left(2\nu+p+1\right)}{\Gamma\left(2\nu\right)}\ {}_3F_2\left(\begin{array}{c} -n,\ p+2,\ -p-1 \\ 2\nu,\quad 1 \end{array}\right).
\end{aligned}
$$

Here, the terminating generalized hypergeometric series ${}_3F_2\left(1\right)$ are related to the Hahn and Chebyshev polynomials of a discrete variable [39], [60]. (See Eqs. (3.11) and (A.1) below, we usually omit the argument of the hypergeometric series ${}_3F_2$ if it is equal to 1.) Two more forms occur if one takes one of the radial wave functions from (2.4) and another one from (2.10). We leave the details to the reader.

The averages of r^p for the relativistic hydrogen atom were evaluated by Davis [15] in a form which is slightly different from our equations (3.4) and (3.7); see also [3] and Ref. [60] for a simple proof of the second formula including evaluation of the corresponding integral of the product of two Laguerre polynomials:

$$
\begin{aligned}
&\int_0^\infty e^{-x}x^{\alpha+s}\ L_n^{\alpha}\left(x\right)L_m^{\beta}\left(x\right)\ dx \qquad (3.10)\\
&\quad = \left(-1\right)^{n-m}\frac{\Gamma\left(\alpha+s+1\right)\Gamma\left(\beta+m+1\right)\Gamma\left(s+1\right)}{m!\left(n-m\right)!\,\Gamma\left(\beta+1\right)\Gamma\left(s-n+m+1\right)} \\
&\quad\times\ {}_3F_2\left(\begin{array}{c} -m,\ s+1,\ \beta-\alpha-s \\ \beta+1,\quad n-m+1 \end{array}\right),\qquad n\geq m.
\end{aligned}
$$

(The limit $c\rightarrow\infty$ of the integral A_p is discussed in [60].) Equations (3.5)–(3.6) and (3.8)–(3.9), which we have not been able to find in the available literature, can be derived in a similar fashion.

It does not appear to have been noticed that the corresponding ${}_3F_2$ functions can be expressed in terms of Hahn polynomials:

$$h_n^{(\alpha,\ \beta)}(x,N)=(-1)^n\,\frac{\Gamma(N)\,(\beta+1)_n}{n!\,\Gamma(N-n)}\ {}_3F_2\left(\begin{array}{c}-n,\ \alpha+\beta+n+1,\ -x\\ \beta+1,\quad 1-N\end{array}\right). \tag{3.11}$$

The ease of handling of these matrix elements for the discrete levels is greatly increased if use is made of the known properties of these polynomials [20], [39], and [40].

For example, the difference-differentiation formulas (4.34)–(4.35) of Ref. [60] (see also (A.5) below) take the following convenient form

$$\begin{aligned}\frac{p(p+1)}{n+2\nu}\ {}_3F_2\left(\begin{array}{c}1-n,\ -p,\ p+1\\ 2\nu+1,\quad 2\end{array}\right)&=\frac{p(p+1)}{2\nu+1}\ {}_3F_2\left(\begin{array}{c}1-n,\ 1-p,\ p+2\\ 2\nu+2,\quad 2\end{array}\right)\\ &={}_3F_2\left(\begin{array}{c}-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{array}\right)-{}_3F_2\left(\begin{array}{c}1-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{array}\right)\end{aligned} \tag{3.12}$$

in terms of the generalized hypergeometric functions. (Another proof of these identities is given in the appendix A.) As a result, the linear relation holds [51], [1]

$$2\kappa\,(A_p-\varepsilon B_p)-(p+1)\,(B_p-\varepsilon A_p)=4\mu C_p, \tag{3.13}$$

and we can rewrite (3.4)–(3.5) in the following matrix form

$$\begin{aligned}&2\,(p+1)\,a\mu\,(2a\beta)^p\ \frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)}\left(\begin{array}{c}A_p\\ B_p\end{array}\right) \qquad (3.14)\\ &=\left(\begin{array}{cc}\gamma_1 & \gamma_2\\ \delta_1 & \delta_2\end{array}\right)\left(\begin{array}{c}{}_3F_2\left(\begin{array}{c}1-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{array}\right)\\ {}_3F_2\left(\begin{array}{c}-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{array}\right)\end{array}\right)\qquad (p\neq-1),\end{aligned}$$

where

$$\gamma_1=(\mu+a\kappa)\,(a\,(2\varepsilon\kappa+p+1)-2\varepsilon\mu)\,,\qquad \gamma_2=(\mu-a\kappa)\,(a\,(2\varepsilon\kappa+p+1)+2\varepsilon\mu)\,, \tag{3.15}$$

$$\delta_1=(\mu+a\kappa)\,(a\,(2\kappa+\varepsilon\,(p+1))-2\mu)\,,\qquad \delta_2=(\mu-a\kappa)\,(a\,(2\kappa+\varepsilon\,(p+1))+2\mu)\,. \tag{3.16}$$

This representation of integrals A_p and B_p involves the Chebyshev polynomials of a discrete variable $h_p^{(0,\ 0)}(x,-2\nu)$ at $x=n,\ n-1$ only; see also equation (3.6) for C_p. The corresponding dual Hahn polynomials [39] may be considered as difference analogs of the Laguerre polynomials in equation (2.10) for the relativistic radial functions.

4. Inversion Formulas

Due to the symmetry of the hypergeometric functions in (3.4)–(3.6) under the transformation $p\rightarrow-p-1$, one gets

$$A_{-p-1}=(2a\beta)^{2p+1}\ \frac{\Gamma(2\nu-p)}{\Gamma(2\nu+p+1)}\frac{\left(\left(1+\varepsilon^2\right)p+\varepsilon^2\right)A_p-(2p+1)\,\varepsilon B_p}{\left(1-\varepsilon^2\right)p}, \tag{4.1}$$

$$B_{-p-1} = (2a\beta)^{2p+1} \ \frac{\Gamma(2\nu - p)}{\Gamma(2\nu + p + 1)} \frac{(2p+1)\,\varepsilon A_p - ((1+\varepsilon^2)\,p + 1)\,B_p}{(1-\varepsilon^2)\,p}, \tag{4.2}$$

$$C_{-p-1} = (2a\beta)^{2p+1} \ \frac{\Gamma(2\nu - p)}{\Gamma(2\nu + p + 1)} \ C_p. \tag{4.3}$$

(These relations allow us to evaluate all the convergent integrals with $p \le -2$.) Indeed,

$$A_{-p-1} - \varepsilon B_{-p-1} = (2a\beta)^{2p+1} \ \frac{\Gamma(2\nu - p)}{\Gamma(2\nu + p + 1)} \left(A_p - \varepsilon B_p\right), \tag{4.4}$$

$$B_{-p-1} - \varepsilon A_{-p-1} = -\frac{p+1}{p} \left(2a\beta\right)^{2p+1} \ \frac{\Gamma(2\nu - p)}{\Gamma(2\nu + p + 1)} \left(B_p - \varepsilon A_p\right), \tag{4.5}$$

which gives the first two equations, if $B_p \neq \varepsilon A_p$ and $p \neq 0, -1$. The last one follows from (3.6). Special cases $p = 0, -1$ of (4.4)–(4.5) are simply identity (6.16) and Fock's virial theorem (6.13), respectively. In view of our formulas (3.4)–(3.5), equation $B_p = \varepsilon A_p$ occurs only when $p = 0$ or $n = 0$.

The symmetry of the hypergeometric functions in (3.7)–(3.9) under another reflection $p \to -p-3$ gives

$$\begin{aligned} A_{-p-3} &= (2a\beta)^{2p+3} \ \frac{\Gamma(2\nu - p - 2)}{\Gamma(2\nu + p + 3)} \\ &\times \left(\frac{4\mu^2 (2p+3) + (p+2)\left(4\nu^2 + (p+1)(p+2)\right)}{p+2} \ A_p \right. \\ &\left. \quad - 2\kappa (2p+3) \ B_p - 8\kappa\mu \frac{2p+3}{p+2} \ C_p \right), \end{aligned} \tag{4.6}$$

$$\begin{aligned} B_{-p-3} &= (2a\beta)^{2p+3} \ \frac{\Gamma(2\nu - p - 2)}{\Gamma(2\nu + p + 3)} \\ &\times \left(-2\kappa (2p+3) \ A_p + \left(4\nu^2 + (p+1)(p+2)\right) \ B_p \right. \\ &\left. \quad + 4\mu (2p+3) \ C_p \right), \end{aligned} \tag{4.7}$$

$$\begin{aligned} C_{-p-3} &= (2a\beta)^{2p+3} \ \frac{\Gamma(2\nu - p - 2)}{\Gamma(2\nu + p + 3)} \\ &\times \left(2\kappa\mu \frac{2p+3}{p+2} \ A_p - \mu (2p+3) \ B_p \right. \\ &\left. \quad - \frac{4\mu^2 (2p+3) + (p+1)\left(4\nu^2 - (p+2)^2\right)}{p+2} \ C_p \right) \end{aligned} \tag{4.8}$$

as a result of elementary matrix multiplications. These relations can be used for all the convergent integrals with $p \le -3$. Further details are left to the reader.

The corresponding single two-term nonrelativistic relation was found by Pasternack [41], [42] (see also [51] and references therein). We have been unable to find the relativistic matrix identities (4.1)–(4.3) and (4.6)–(4.8) in the available literature (see Eq. (18) of Ref. [3] as the closest analog).

5. Recurrence Relations

A set of useful recurrence relations between the relativistic matrix elements was derived by Shabaev [51] (see also [18], [62], [56], and [1]) on the basis of hypervirial theorem:

$$2\kappa A_p - (p+1)\, B_p = 4\mu C_p + 4\beta\varepsilon C_{p+1}, \tag{5.1}$$

$$2\kappa B_p - (p+1)\, A_p = 4\beta C_{p+1}, \tag{5.2}$$

$$\mu B_p - (p+1)\, C_p = \beta\left(A_{p+1} - \varepsilon B_{p+1}\right). \tag{5.3}$$

Linear relation (3.13) and convenient recurrence formulas

$$\begin{aligned} A_{p+1} = & -(p+1)\,\frac{4\nu^2\varepsilon + 2\kappa\,(p+2) + \varepsilon\,(p+1)\,(2\kappa\varepsilon + p + 2)}{4\left(1-\varepsilon^2\right)(p+2)\,\beta\mu}\; A_p \\ & + \frac{4\mu^2\,(p+2) + (p+1)\,(2\kappa\varepsilon + p + 1)\,(2\kappa\varepsilon + p + 2)}{4\left(1-\varepsilon^2\right)(p+2)\,\beta\mu}\; B_p, \end{aligned} \tag{5.4}$$

$$\begin{aligned} B_{p+1} = & -(p+1)\,\frac{4\nu^2 + 2\kappa\varepsilon\,(2p+3) + \varepsilon^2\,(p+1)\,(p+2)}{4\left(1-\varepsilon^2\right)(p+2)\,\beta\mu}\; A_p \\ & + \frac{4\mu^2\varepsilon\,(p+2) + (p+1)\,(2\kappa\varepsilon + p + 1)\,(2\kappa + \varepsilon\,(p+2))}{4\left(1-\varepsilon^2\right)(p+2)\,\beta\mu}\; B_p, \end{aligned} \tag{5.5}$$

$$C_{p+1} = \frac{1}{4\mu}\left(2\kappa + \varepsilon\,(p+2)\right)\; A_{p+1} - \frac{1}{4\mu}\left(2\kappa\varepsilon + p + 2\right)\; B_{p+1} \tag{5.6}$$

are obtained from these equations (see [51], [56], and [1] for more details). Their connections with the theory of generalized hypergeometric functions will be discussed elsewhere.

6. Special Expectation Values and Their Applications

The Sommerfeld–Dirac formula (2.8) is derived for a point charge atomic nucleus with infinite mass and no internal structure (electron moving in static Coulomb field). In reality, the electron's mass is not negligibly small compared with the nuclear mass and one has to consider the effect of nuclear motion on the energy levels. Actual nuclei have a finite size and possess some internal structure, such as an internal angular momentum or spin, a magnetic dipole moment, and a small electric quadrupole moment associated with the spin, which also affect the energy levels. Radiative corrections are introduced by the quantization of the electromagnetic radiation field. (See [8], [11], [52], [53], [54], [55], [63], and [58] and references therein for more details.) Calculations of the real energy levels of the high-Z one-electron systems with the help of the perturbation theory require special relativistic matrix elements.

From the explicit expressions (3.4)–(3.9) one can derive the following special matrix elements:

$$\begin{aligned} A_2 &= \left\langle r^2 \right\rangle = \frac{5n\,(n+2\nu) + 4\nu^2 + 1 - \varepsilon\kappa\,(2\varepsilon\kappa + 3)}{2\,(a\beta)^2} \\ &= \frac{2\kappa^2\varepsilon^4 + 3\kappa\varepsilon^3 + \left(3\mu^2 - \nu^2 - 1\right)\varepsilon^2 - 3\kappa\varepsilon - \nu^2 + 1}{2\beta^2\left(1-\varepsilon^2\right)^2}, \end{aligned} \tag{6.1}$$

$$A_1 = \langle r \rangle = \frac{3\varepsilon\mu^2 - \kappa\left(1-\varepsilon^2\right)(1+\varepsilon\kappa)}{2\beta\mu\left(1-\varepsilon^2\right)}, \tag{6.2}$$

$$A_0 = \langle 1 \rangle = 1, \tag{6.3}$$

$$\begin{aligned} A_{-1} &= \left\langle \frac{1}{r} \right\rangle = \frac{\beta}{\mu\nu}\left(1-\varepsilon^2\right)\left(\varepsilon\nu + \mu\sqrt{1-\varepsilon^2}\right) \\ &= \frac{m^2c^4 - E^2}{m^2c^4}\left(\frac{E}{Ze^2} + \sqrt{\frac{m^2c^4 - E^2}{\hbar^2c^2\kappa^2 - Z^2e^4}}\right), \end{aligned} \tag{6.4}$$

$$A_{-2} = \left\langle \frac{1}{r^2} \right\rangle = \frac{2a^3\beta^2\kappa\left(2\varepsilon\kappa - 1\right)}{\mu\nu\left(4\nu^2 - 1\right)}, \tag{6.5}$$

$$A_{-3} = \left\langle \frac{1}{r^3} \right\rangle = 2\left(a\beta\right)^3 \frac{3\varepsilon^2\kappa^2 - 3\varepsilon\kappa - \nu^2 + 1}{\nu\left(\nu^2-1\right)\left(4\nu^2-1\right)}. \tag{6.6}$$

(Note that A_{-3} exists only if $|\kappa| \geq 2$ [51].) The average distance between the electron and the nucleus $\overline{r} = \langle r \rangle$ is given by A_1. The mean square deviation of the nucleus-electron separation is $\overline{(r-\overline{r})^2} = A_2 - (A_1)^2$. The energy eigenvalue $\langle E \rangle$, mean radius $\langle r \rangle$ and mean square radius $\langle r^2 \rangle$ are frequently used when making comparisons of wave functions computed by different approximation methods. The integrals A_1 and A_2 have been evaluated in [23], [13], [44], and [60] (see also Ref. [3] for closed-form expressions for $\{A_p\}_{p=-6}^{5}$). Matrix element A_{-3} appears in calculation of the electric quadrupole hyperfine splitting [43], [52], and [56]. Integrals A_p are also part of the expression for the effective electrostatic potential for the relativistic hydrogenlike atom [60].

$$\begin{aligned} B_2 &= \left\langle \beta r^2 \right\rangle = \frac{\varepsilon}{2\left(a\beta\right)^2}\left(5n\left(n+2\nu\right) + 2\nu^2 + 1 - 3\varepsilon\kappa\right) \\ &= \varepsilon\frac{3\kappa\varepsilon^3 + \left(5\mu^2 + 3\nu^2 - 1\right)\varepsilon^2 - 3\kappa\varepsilon - 3\nu^2 + 1}{2\beta^2\left(1-\varepsilon^2\right)^2}, \end{aligned} \tag{6.7}$$

$$B_1 = \langle \beta r \rangle = \frac{3\varepsilon^2\mu^2 - \left(1-\varepsilon^2\right)\left(\varepsilon\kappa + \nu^2\right)}{2\beta\mu\left(1-\varepsilon^2\right)}, \tag{6.8}$$

$$B_0 = \langle \beta \rangle = \varepsilon = \frac{E}{mc^2}, \tag{6.9}$$

$$B_{-1} = \left\langle \frac{\beta}{r} \right\rangle = \frac{\beta a^2}{\mu} = \frac{m^2c^4 - E^2}{Ze^2mc^2}, \tag{6.10}$$

$$B_{-2} = \left\langle \frac{\beta}{r^2} \right\rangle = \frac{2a^3\beta^2\left(2\nu^2 - \varepsilon\kappa\right)}{\mu\nu\left(4\nu^2-1\right)}, \tag{6.11}$$

$$B_{-3} = \left\langle \frac{\beta}{r^3} \right\rangle = 2\left(a\beta\right)^3\varepsilon\frac{1 + 2\nu^2 - 3\varepsilon\kappa}{\nu\left(\nu^2-1\right)\left(4\nu^2-1\right)}. \tag{6.12}$$

The integral B_0 appears in the virial theorem for the Dirac equation in a Coulomb field,

$$E = mc^2 \langle \beta \rangle, \tag{6.13}$$

established by Fock [22] and then developed by many authors (see [11], [12], [45], [32], [49], [17], [36], [47], [18], [48], [21], [24], [51], and [56] and references therein). Relation (6.13) can also be obtained with the help of the Hellmann–Feynman theorem,

$$\frac{\partial E}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle \tag{6.14}$$

(see [18], [36], [5], and [6] and references therein), if applied to the mass parameter [1], [56]. This theorem implies two more relations

$$\frac{\partial E}{\partial Z}=-e^{2}\left\langle \frac{1}{r}\right\rangle =-e^{2}A_{-1},\qquad \frac{\partial E}{\partial \kappa}=2\hbar cC_{-1}. \tag{6.15}$$

The following identities hold

$$A_{-1}-\varepsilon B_{-1}=\frac{a^{3}\beta}{\nu}=\frac{1}{\beta}\left(\mu B_{-2}+C_{-2}\right) \tag{6.16}$$

by (5.3). The integral B_{-1} is evaluated in [11] and A_{-1}, A_{-2}, B_{-2}, C_{-2}, and A_{-3} are given in [51] (see also [56]).

The relativistic recoil corrections to the energy levels, when nuclear motion is taken into consideration, require matrix elements A_{-2}, B_{-1} and C_{-2} (see [11], [53], [54], and [1] and references therein).

$$\begin{aligned} C_{2} &= \frac{\kappa a^{2}\left(3n\left(n+2\nu\right)+2\nu^{2}+1\right)-3\mu^{2}\varepsilon}{4\mu\left(a\beta\right)^{2}} \\ &= \frac{\kappa\left(1-\varepsilon^{2}\right)\left(1-\nu^{2}\right)+3\varepsilon\mu^{2}\left(\varepsilon\kappa-1\right)}{4\mu\beta^{2}\left(1-\varepsilon^{2}\right)}, \end{aligned} \tag{6.17}$$

$$C_{1}=\frac{2\varepsilon\kappa-1}{4\beta}=\frac{\hbar}{4m^{2}c^{3}}\left(2\kappa E-mc^{2}\right), \tag{6.18}$$

$$C_{0}=\frac{\kappa}{2\mu}\left(1-\varepsilon^{2}\right)=\frac{\hbar c\kappa}{2Ze^{2}}\frac{m^{2}c^{4}-E^{2}}{m^{2}c^{4}}, \tag{6.19}$$

$$\begin{aligned} C_{-1} &= \frac{\kappa}{2\mu\nu}a^{3}\beta=\frac{a\beta}{\nu}C_{0} \\ &= \frac{\hbar\kappa}{2Ze^{2}m^{2}c^{3}}\frac{\left(m^{2}c^{4}-E^{2}\right)^{3/2}}{\left(\hbar^{2}c^{2}\kappa^{2}-Z^{2}e^{4}\right)^{1/2}}, \end{aligned} \tag{6.20}$$

$$C_{-2}=\frac{a^{3}\beta^{2}\left(2\varepsilon\kappa-1\right)}{\nu\left(4\nu^{2}-1\right)}=\frac{4\left(a\beta\right)^{3}C_{1}}{\nu\left(4\nu^{2}-1\right)}, \tag{6.21}$$

$$C_{-3}=\left(a\beta\right)^{3}\frac{\kappa\left(1-\varepsilon^{2}\right)\left(1-\nu^{2}\right)+3\varepsilon\mu^{2}\left(\varepsilon\kappa-1\right)}{\mu\nu\left(\nu^{2}-1\right)\left(4\nu^{2}-1\right)}=\frac{4\left(a\beta\right)^{5}C_{2}}{\nu\left(\nu^{2}-1\right)\left(4\nu^{2}-1\right)}. \tag{6.22}$$

The integrals C_0, C_1, and B_{-1} are computed in [24]. In view of (6.10) and (6.19), respectively (6.5) and (6.21), the following simple relations hold

$$C_{0}=\frac{\kappa}{2\beta}B_{-1},\qquad A_{-2}=\frac{2\kappa}{\mu}C_{-2}=\frac{8\left(a\beta\right)^{3}\kappa}{\mu\nu\left(4\nu^{2}-1\right)}C_{1}. \tag{6.23}$$

The last but one was originally found in [12].

The integral C_1 occurs in calculations of the bound-electron g factor (the anomalous Zeeman effect in the presence of an external homogeneous static magnetic field) [33], [47], [64], [56], and [57]. The matrix element C_{-1} has also been found by the Hellmann–Feynman theorem (6.15). The integral C_{-2} appears in calculation of the magnetic dipole hyperfine splitting [10], [12], [35], [21], [43], [47], and [52].

The author hopes that the rest of matrix elements will also be useful in the current theory of hydrogenlike heavy ions and other exotic relativistic Coulomb systems. Professor Shabaev kindly pointed out that the formulas derived in this paper can be used in calculations with hydrogenlike wave functions where a high precision is required.

In Table 1, we list the expectation values for the $1s_{1/2}$ state, when $n = n_r = 0$, $l = 0$, $j = 1/2$, and $\kappa = -1$. The corresponding radial wave functions are given by Eq. (2.14).

Table 1. Expectation values for the $1s_{1/2}$ state.

p	A_p	B_p	C_p
2	$\frac{1}{2}\left(\frac{a_0}{Z}\right)^2 (\nu_1+1)(2\nu_1+1)$	$\frac{1}{2}\left(\frac{a_0}{Z}\right)^2 \nu_1(\nu_1+1)(2\nu_1+1)$	$-\frac{\lambda a_0}{4Z}(\nu_1+1)(2\nu_1+1)$
1	$\frac{a_0}{2Z}(2\nu_1+1)$	$\frac{a_0}{2Z}\nu_1(2\nu_1+1)$	$-\frac{\lambda}{4}(2\nu_1+1)$
0	1	ν_1	$-\frac{\lambda Z}{2a_0}$
-1	$\frac{Z}{a_0\nu_1}$	$\frac{Z}{a_0}$	$-\left(\frac{Z}{a_0}\right)^2 \frac{\lambda}{2\nu_1}$
-2	$\left(\frac{Z}{a_0}\right)^2 \frac{2}{\nu_1(2\nu_1-1)}$	$\left(\frac{Z}{a_0}\right)^2 \frac{2}{(2\nu_1-1)}$	$-\left(\frac{Z}{a_0}\right)^3 \frac{\lambda}{\nu_1(2\nu_1-1)}$
-3	$\left(\frac{Z}{a_0}\right)^3 \frac{2}{\nu_1(\nu_1-1)(2\nu_1-1)}$	$\left(\frac{Z}{a_0}\right)^3 \frac{2}{(\nu_1-1)(2\nu_1-1)}$	$-\left(\frac{Z}{a_0}\right)^4 \frac{\lambda}{\nu_1(\nu_1-1)(2\nu_1-1)}$

In the table, $\varepsilon_1 = \nu_1 = \sqrt{1-\mu^2} = \sqrt{1-(\alpha Z)^2}$, $\alpha = e^2/\hbar c$ is the Sommerfeld fine structure constant, $a_0 = \hbar^2/me^2$ is the Bohr radius, and $\lambda = \hbar/mc$ is the Compton wavelength. The relations

$$B_p = \varepsilon_1\ A_p, \qquad C_p = -\frac{\lambda Z}{2a_0}\ A_p, \qquad A_p = \left(\frac{a_0}{2Z}\right)^p \frac{\Gamma(2\nu_1+p+1)}{\Gamma(2\nu_1+1)} \tag{6.24}$$

(for all the suitable integers $p > -2\nu_1 - 1 > -3$) follow directly from (3.4), (3.5) and (3.7), (3.9). (The formal expressions for A_{-3}, B_{-3}, and C_{-3}, when the integrals diverge, are included into the table for "completeness"; see Ref. [1] for more details.) The reflection relation (4.3) holds for all the convergent integrals A_p, B_p, and C_p.

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Appendix A. Generalized Hypergeometric Series

The generalized hypergeometric series is defined as follows [4], [20]

$$\begin{aligned} &{}_pF_q\left(a_1,\ a_2,\ \dots,\ a_p;\ b_1,\ b_2,\ \dots,\ b_q;\ z\right) \\ &= {}_pF_q\left(\begin{array}{c} a_1,\ a_2,\ \dots,\ a_p \\ b_1,\ b_2,\ \dots,\ b_q \end{array};\ z\right) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n \cdots (a_p)_n\ z^n}{(b_1)_n (b_2)_n \cdots (b_q)_n\, n!}, \end{aligned} \tag{A.1}$$

where $(a)_n = a(a+1)\dots(a+n-1) = \Gamma(a+n)/\Gamma(a)$. In this paper we always have $p=3$, $q=2$, $z=1$, and a_1 is a negative integer when the series terminates. The Laguerre polynomials are given by [20], [39], [40]:

$$L_n^{\alpha}(x) = \frac{\Gamma(\alpha+n+1)}{n!\,\Gamma(\alpha+1)}\ {}_1F_1\left(\begin{array}{c} -n \\ \alpha+1 \end{array};\ x\right). \tag{A.2}$$

The required identity (3.12) can be derived from the theory of classical polynomials in the following fashion. Let us start from the difference equation for the Hahn polynomials $y_m = h_m^{(\alpha,\,\beta)}(x,N)$ [39]:

$$\left(\sigma(x)\nabla + \tau(x)\right)\Delta y_m + \lambda_m y_m = 0, \tag{A.3}$$

where $\Delta f(x) = \nabla f(x+1) = f(x+1) - f(x)$ and

$$\begin{aligned} \sigma(x) &= x(\alpha+N-x), \\ \tau(x) &= (\beta+1)(N-1) - (\alpha+\beta+2)x, \\ \lambda_m &= m(\alpha+\beta+m+1), \end{aligned} \tag{A.4}$$

and use the familiar difference-differentiation formula:

$$\Delta h_m^{(\alpha,\,\beta)}(x,N) = (\alpha+\beta+m+1)\,h_{m-1}^{(\alpha+1,\,\beta+1)}(x,N-1). \tag{A.5}$$

As a result,

$$\left(\sigma(x)\nabla + \tau(x)\right)h_{m-1}^{(\alpha+1,\,\beta+1)}(x,N-1) + m h_m^{(\alpha,\,\beta)}(x,N) = 0. \tag{A.6}$$

Letting $\alpha=\beta$ and $\beta\to-1$, one gets

$$\begin{aligned} x(N-x-1)\nabla h_{m-1}^{(0,\,0)}(x,N-1) &= -m\lim_{\beta\to-1} h_m^{(\beta,\,\beta)}(x,N) \\ &= (-1)^m m(m-1)\frac{\Gamma(N-1)}{\Gamma(N-m)} x\ {}_3F_2\left(\begin{array}{c} 1-m,\ m,\ 1-x \\ 2,\quad 2-N \end{array}\right) \end{aligned} \tag{A.7}$$

by (3.11). The last identity takes the form (3.12), if the Chebyshev polynomials of a discrete variable $h_{m-1}^{(0,\,0)}(x,N-1)$ are replaced by the corresponding generalized hypergeometric functions. (Use of (A.5) in (A.7) gives the special ${}_3F_2$ transformation.)

Appendix B. Dirac Matrices and Inner Product

We use the standard representations of the Dirac and Pauli matrices:

$$\boldsymbol{\alpha} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \tag{B.1}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{B.2}$$

with

$$\mathbf{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{B.3}$$

The inner product of two Dirac (bispinor) wave functions

$$\psi = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{v}_1 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}, \qquad \phi = \begin{pmatrix} \mathbf{u}_2 \\ \mathbf{v}_2 \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} \tag{B.4}$$

is defined as a scalar quantity

$$\begin{aligned} \langle \psi,\ \phi \rangle &= \int_{\mathbf{R}^3} \psi^\dagger \phi \ dv = \int_{\mathbf{R}^3} \left(\mathbf{u}_1^\dagger \mathbf{u}_2 + \mathbf{v}_1^\dagger \mathbf{v}_2 \right) \ dv \\ &= \int_{\mathbf{R}^3} \left(\psi_1^* \phi_1 + \psi_2^* \phi_2 + \psi_3^* \phi_3 + \psi_4^* \phi_4 \right) \ dv \end{aligned} \tag{B.5}$$

and the corresponding expectation values of a matrix operator A are given by

$$\langle A \rangle = \langle \psi,\ A\psi \rangle . \tag{B.6}$$

From this definition one gets

$$\langle r^p \rangle = A_p, \qquad \langle \beta r^p \rangle = B_p, \qquad \langle i\boldsymbol{\alpha}\mathbf{n}\beta r^p \rangle = -2C_p, \tag{B.7}$$

where the integrals A_p, B_p, and C_p are given by (3.1)–(3.3), respectively.

Indeed, the first relation is derived, for example, in Ref. [60] and the second one can be obtained by integrating the identity

$$\begin{aligned} r^p \psi^\dagger \beta \psi &= r^p \left(\boldsymbol{\varphi}^\dagger,\ \boldsymbol{\chi}^\dagger \right) \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{\varphi} \\ \boldsymbol{\chi} \end{pmatrix} = r^p \left(\boldsymbol{\varphi}^\dagger,\ \boldsymbol{\chi}^\dagger \right) \begin{pmatrix} \boldsymbol{\varphi} \\ -\boldsymbol{\chi} \end{pmatrix} \\ &= r^p \left(\boldsymbol{\varphi}^\dagger \boldsymbol{\varphi} - \boldsymbol{\chi}^\dagger \boldsymbol{\chi} \right) = r^p \left(\mathcal{Y}^\dagger \mathcal{Y} \right) \left(F^2 - G^2 \right) \end{aligned} \tag{B.8}$$

(we leave details to the reader) in a similar fashion.

In the last case, we start from the matrix identity

$$\left(\boldsymbol{\alpha}\mathbf{n} \right) \beta \psi = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma}\mathbf{n} \\ \boldsymbol{\sigma}\mathbf{n} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\varphi} \\ -\boldsymbol{\chi} \end{pmatrix} = \begin{pmatrix} -\left(\boldsymbol{\sigma}\mathbf{n} \right)\ \boldsymbol{\chi} \\ \left(\boldsymbol{\sigma}\mathbf{n} \right)\ \boldsymbol{\varphi} \end{pmatrix} \tag{B.9}$$

and use the Ansatz [60]

$$\boldsymbol{\varphi} = \boldsymbol{\varphi}\left(\mathbf{r} \right) = \mathcal{Y}\left(\mathbf{n} \right)\ F\left(r \right), \qquad \boldsymbol{\chi} = \boldsymbol{\chi}\left(\mathbf{r} \right) = -i \left(\left(\boldsymbol{\sigma}\mathbf{n} \right) \mathcal{Y}\left(\mathbf{n} \right) \right)\ G\left(r \right), \tag{B.10}$$

where $\mathbf{n} = \mathbf{r}/r$ and $\mathcal{Y} = \mathcal{Y}_{jm}^{\pm}\left(\mathbf{n} \right)$ are the spinor spherical harmonics given by (2.3). As a result,

$$\begin{aligned} & i r^p \psi^\dagger \left(\left(\boldsymbol{\alpha}\mathbf{n} \right) \beta \psi \right) \\ &= i r^p \left(\boldsymbol{\varphi}^\dagger,\ \boldsymbol{\chi}^\dagger \right) \begin{pmatrix} -\left(\boldsymbol{\sigma}\mathbf{n} \right)\ \boldsymbol{\chi} \\ \left(\boldsymbol{\sigma}\mathbf{n} \right)\ \boldsymbol{\varphi} \end{pmatrix} = i r^p \left(F\mathcal{Y}^\dagger,\ iG\mathcal{Y}^\dagger \left(\boldsymbol{\sigma}\mathbf{n} \right) \right) \begin{pmatrix} i\mathcal{Y}G \\ \left(\boldsymbol{\sigma}\mathbf{n} \right) \mathcal{Y}F \end{pmatrix} \\ &= -r^p \left(\mathcal{Y}^\dagger \mathcal{Y} \right) FG - r^p \left(\mathcal{Y}^\dagger \left(\boldsymbol{\sigma}\mathbf{n} \right)^2 \mathcal{Y} \right) FG = -2r^p \left(\mathcal{Y}^\dagger \mathcal{Y} \right) FG \end{aligned} \tag{B.11}$$

with the help of the familiar identity $\left(\boldsymbol{\sigma}\mathbf{n} \right)^2 = \mathbf{n}^2 = \mathbf{1}$. Integration over $\mathbf{R}^3$ in the spherical coordinates completes the proof.

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